Indian J. Phys. **75A** (1), 61-63 (2001)

IJP A
— an international journal

On relativistic study of a simple one-dimensional model of the field emission microscope

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Abstract : The paper is concerned with a relativistic generalization of a simple one-dimensional model of the field emission microscope studied non-relativistically by M Steslicka The bulk potentials are represented by δ-wells. Avoiding the normalization problem, we derived the exact energy expression for virtual surface states by following an approach due to Steslicka, Davison and Roy and Roy. We have carried out some quantitative explorations of our numerical results and discussed critically these investigations in the light of corresponding nonrelativistic findings

Keywords . Field emission microscope, relativistic study, one-dimensional model

PACS Nos. 61 16 Fk, 03 65 Pm, 73 20 At

1. Introduction

Virtual surface states, *i.e.* Surface States (SS) in the presence of an external negative electric field have gained considerable importance during about the last decade. The pioneering work in this area is that due to Davison *et al* [1] and the subsequent work was that due to Steslicka and Parkal [2]. All these treatments were carried out nonrelativistically. For solids with heavy atoms, the surface states (as well as bulk states) require to be treated relativistically. Several authors carried out relativistic [3-7] work considering the semi-infinite crystal model. The purpose of the present paper is to report a relativistic treatment assuming a simple one-dimensional model applicable in the field emission microscope studied by Steslicka and Parkal [2]. The advantages of our model are the following : we avoid the normalization problem in a natural way and in addition, we derive the energy expression for virtual SS in an analytical form. Our treatment is based on an approach due to Steslicka and Davison [5].

2. The model

We assume that the field emission microscope can be represented by a simple model shown in Figure 1. The bulk potential is expressed by δ-wells (attractive). The potential model is

$$V(x) = (-p/a)\sum_{n=0}^{\infty}\delta(x+na), \quad \text{for } x < a \tag{1}$$

$$V(x) = V_0 - F.x \ , \quad \text{for } 0 < x < d, \tag{2}$$

where the crystal potential p, a and v represent the crystal δ-wells, the lattice constant and the work function respectively, F is the intensity of the applied field. Hartree atomic units ($h = m = e = 1$) are used in this paper.

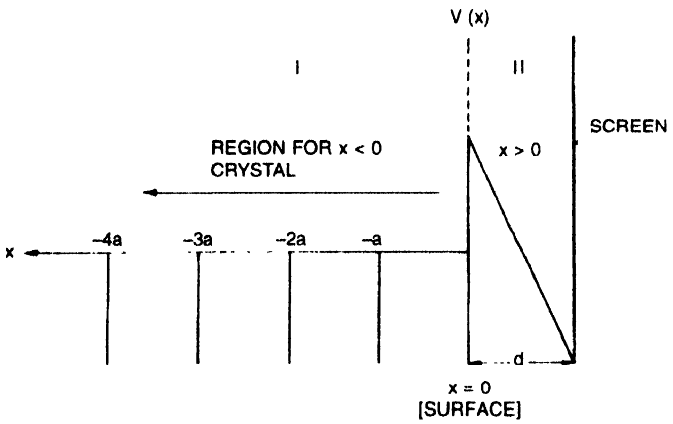

Figure 1. Model of field emission microscope, Crystal ($x < 0$) is represented by Kronig-Penny model and the screen ($x = d$) by infinitely high potential wall.

3. Wave functions in various regions

Region I : The wavefunction in region 1 is to be obtained on the basis of one-dimensional Dirac equation [5].

$$\frac{d^2\Phi(x)}{dx^2} = -\rho_v^2\,\Phi(x), \tag{3}$$

where $\rho_v^2 = \{\varepsilon - V(x)\}\{\varepsilon - V(x) + 2mc^2\}\ \hbar^2 c^2$,

m = rest mass of the electron, c = velocity of light, $\varepsilon = E - mc^2$, E = total (relativistic) energy of the electron.

In the region 1, the wave function Φ_I is given by [3]

$$\Phi_I = \alpha_1\left[\exp\{i\rho(x+a)\} + \lambda_R \exp\{-i\rho(x+a)\}\right].\exp(i\mu a), \tag{4}$$

where λ_R is given by Steslicka and Thakkar [3]

$$\lambda_R = \{1 - \exp i(\rho+\mu)a\}/\{\exp - i(\rho-\mu)a - 1\}. \tag{5}$$

Region 2 : Taking note of $V(x)$ given by (2), the equation to be satisified by the wave function in the region 2, can be written as :

$$\frac{d^2\Phi_{II}}{dx^2} + (C_0 + C_1 x + C_2 x^2)\Phi_{II} = 0, \tag{6}$$

where $C_0 = (\varepsilon - V_0)\{(\varepsilon - V_0) + 2C^2\}\Big|\,C^2$;

$$C_1 = \left[2F\{(V_0 - \varepsilon) - C^2\}\right]\Big|\,C^2\,;\ C_2 = F^2/C^2. \tag{7}$$

The values of C_0 and C_1, will be in general, be much larger than the value of C_2, especially for fields which are not too large. Hence taking $C_2 = 0$, we can reduce eq. (6) to the following form

$$\frac{d^2\Phi_{II}}{dx^2} + (C_0 + C_1 x)\Phi_{II} = 0\,. \tag{8}$$

Eq. (8) can be further reduced to the following form

$$\frac{d^2\Phi_{II}}{dz^2} - z\Phi_{II} = 0\,, \tag{9a}$$

$$\text{where } C_1^{2/3} z = -C_0 - C_1 x. \tag{9b}$$

Now eq. (9a) is the well-known Airy's eq. [8]. The general solution of this equation is given by

$$\Phi_{II}(z) = \alpha_2\, A_i(z) + \beta_2 B_i(z)\,, \tag{10}$$

where $A_i(z)$ and $B_i(z)$ are Airy's functions.

As has been discussed by Steslicka, the only solution remains finite for $x > 0$ and hence for $z > 0$, is $A_i(z)$. Thus, the acceptable solution of Φ_{II} is given by

$$\Phi_{II}(z) = \alpha_2\, A_i(z). \tag{11}$$

In addition (cf. Figure 1), the wave function at $x = d$ (the screen of the field emission microscope) is

$$\Phi_{II}(d) = 0. \tag{12}$$

4. Equations for virtual surface state energies and existence conditions

For the model of Figure 1, the boundary condition at $x = 0$ is

$$\Phi_I(x=0) = \Phi_{II}(z=z_0)\,, \tag{13a}$$

$$\left.\frac{d\Phi_I}{dx}\right|_{x=0} = \frac{d\Phi_{II}}{dz}\cdot\left.\frac{dz}{dx}\right|_{x=0} + \frac{2P}{a}\Phi_I(x=0). \tag{13b}$$

Further combining (4), (8) and (13), we have the following results corresponding to δ-well potentials in the bulk regions

$$\exp(i\mu a) = \cos\xi + (\sin\xi/\xi)(\eta_R^a + 2P) \tag{14}$$

$$\text{where, } \xi = \rho a\ ;\ \ \eta_R = \frac{A_i'(z_0)}{A_i(z_0)}\left(\frac{dz}{dx}\right)_{x=0} \tag{15}$$

Now for virtual surface states, the wave vector 'μ ' takes complex values as follows [9].

$$\mu = (n\pi)/a + \delta\ ;\ \delta > 0\,;\ n \text{ is any integer.} \tag{16}$$

The relativistic dispersion relation (Kronig Penny) for the bulk (periodic) region is given by :

$$\cos\mu a = \cos\xi - P.(\sin\xi/\xi). \tag{17}$$

Combining (14), (16) and (17) we get the relativistic virtual surface state energy (SSE) equation of the model of Figure 1

$$\xi\cot\xi = -\{\xi^2 + \eta_{Ra}(\eta_{Ra} + 2P)\}/2P. \tag{18}$$

To derive the existence condition for virtual surface states, we first note that by combining equations (14) with (16) and (17):

$$(-1)^n \sin h\,(a\,\delta) = (\sin\xi/\xi)(P + \eta_{Ra}). \tag{19}$$

Now sign $(\sin\xi/\xi) = (-1)^{n+1}$ for δ- wells.

$$\text{Where, } n\pi \le \xi \le (n+1)\pi \tag{20}$$

According to Steslicka [3] and Roy and Roy [6], we get the relativistic existence condition

$$(P + \eta_R a) < 0 \quad \text{for } \delta\text{- wells.} \tag{21}$$

5. Non-relativistic cases

Our relativistic results (18) and (21) reduce to the nonrelativistic one under the usual limit $c \to \infty$:

$$\xi_0 \cot\xi_0 = (-\xi_0^2/2p) - \left[(\eta)_{NR} a\{(\eta)_{NR} a + 2p\}\right]/2p \tag{22}$$

$$\{(\eta)_{NR} a + p\} < 0 \quad \text{for } \delta\text{- wells.} \tag{23}$$

Equations (22) and (23) together express the nonrelativistic results obtained by Steslicka [2] for the model of Figure 1.

6. Conclusion

In order to compare our relativistic and nonrelativistic results of Steslicka and Parkal with findings of Davison *et al* [1], we calculated the dependence of RSS energy ε and NRSS energy E on the field intensity F. The obtained curve (Figure 2) is in good agreement with their results *i.e.* for lower field values, ε (or E) decreases with increasing F, then reaches minimum at about 3 volt/Å and after passing the minimum, ε (or E) increases with F. We further see that the relativistic SSE are in general higher than the NR ones.

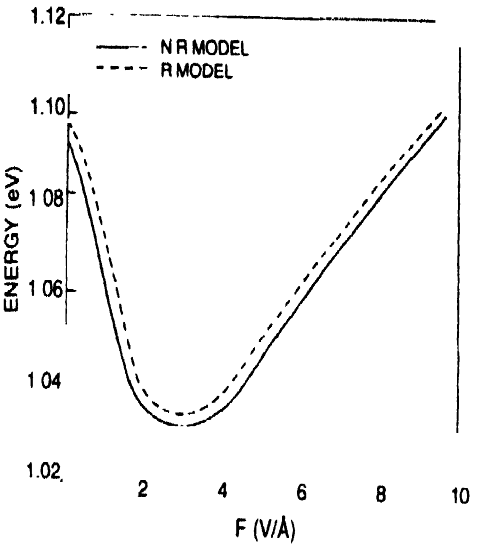

Figure 2. Energy of virtual SS *vs* F curve

Acknowledgments

The author is grateful to Prof. P. K. Mahapatra, Vidyasagar University, India, for a critical reading of the present manuscript and for giving his valuable opinion on its merits.

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